

## Lattice thermal conductivity of ultra high temperature ceramics (UHTC) ZrB<sub>2</sub> and HfB<sub>2</sub> from atomistic simulations

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Ultra high temperature ceramics (UHTC) including ZrB<sub>2</sub> and HfB<sub>2</sub> have a number of properties that make them attractive for applications in extreme environments. One such property is their high thermal conductivity. Computational modeling of these materials will facilitate understanding of fundamental mechanisms, elucidate structure-property relationships, and ultimately accelerate the materials design cycle. Progress in computational modeling of UHTCs however has been limited in part due to the absence of suitable interatomic potentials. Recently, we developed Tersoff style parameterizations of such potentials for both ZrB<sub>2</sub> and HfB<sub>2</sub> appropriate for atomistic simulations. As an application, Green-Kubo molecular dynamics simulations were performed to evaluate the lattice thermal conductivity for single crystals of ZrB<sub>2</sub> and HfB<sub>2</sub>. The atomic mass difference in these binary compounds leads to oscillations in the time correlation function of the heat current, in contrast to the more typical monotonic decay seen in monoatomic materials such as Silicon, for example. Results at room temperature and at elevated temperatures will be reported.